

Product Name: PFI 4

Catalog No.: 5576

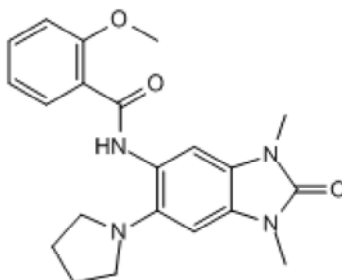
Batch No.: 1

CAS Number: 900305-37-5

IUPAC Name: *N*-[2,3-Dihydro-1,3-dimethyl-2-oxo-6-(1-pyrrolidinyl)-1*H*-benzimidazol-5-yl]-2-methoxybenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₄N₄O₃
Batch Molecular Weight: 380.44
Physical Appearance: Pale green solid
Solubility: DMSO to 50 mM
ethanol to 10 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.3	6.36	14.73
Found	66.4	6.4	14.66

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Potent and selective BRPF1B bromodomain inhibitor (IC_{50} = 172 nM). Exhibits >100-fold selectivity for BRPF1 over a panel of other bromodomains including BRPF2 (BRD1), BRPF3 and BRD4. Disrupts BRPF1 binding to histone H3.3. Cell permeable. Inhibits osteoclastogenesis.

Physical and Chemical Properties:

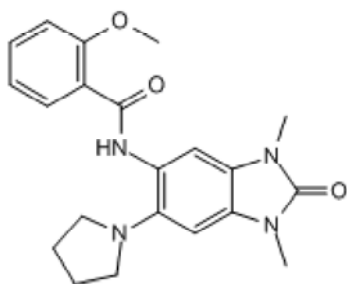
Batch Molecular Formula: $C_{21}H_{24}N_4O_3$

Batch Molecular Weight: 380.44

Physical Appearance: Pale green solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 50 mM

ethanol to 10 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

Licensing Information:

This probe is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the PFI 4 probe summary on the SGC website.

References:

Meier et al (2017) Selective targeting of bromodomains of the bromodomain-PHD fingers family impairs osteoclast differentiation. *ACS Chem.Biol.* **12** 2619. PMID: 28849908.

Demont et al (2014) 1,3-Dimethyl Benzimidazolones are potent, selective inhibitors of the BRPF1 bromodomain. *ACS Med.Chem.Lett.* **5** 1190. PMID: 25408830.

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